CONTENTS

Special Issue: Structure and Bonding of Organic Sulphur Compounds — A Collection of Invited Papers Dedicated to the Memory of Professor Angelo Mangini.

Bonding in selected normal (octet), hypervalent (decet) and super-hypervalent (duodecet) sulfur compounds
E.A. Innes and I.G. Csizmadia (Toronto, Ont., Canada) and Y. Kanada (Tokyo, Japan) 1
The duodecet rule. Part 1. Valence bond structures of oxo and azo species of Si(IV), P(V), S(VI), and Cl(VII)
E.A. Robinson (Mississauga, Ont., Canada) 9
The duodecet rule. Part 2. C–H hydrogen bonding by sulfonyl compounds
E.A. Robinson (Mississauga, Ont., Canada) 29
Bond orders in three-centre bonds: an analytical investigation into the electronic structure of diborane and the three-centre four-electron bonds of hypervalent sulphur
I. Mayer (Budapest, Hungary) 43
Intramolecular sulfur–oxygen interaction in sulfonium compounds and sulfoxides
J.G. Ángyán and R. Daudel (Paris, France), Á. Kucsman (Budapest, Hungary) and I.G. Csizmadia (Toronto, Ont., Canada) 53
Bond orders in three-centre bonds. Part 2. The role of *d*-orbital participation in sulfuranes and related systems
J.G. Ángyán (Budapest, Hungary) 61
Ab initio study of sulfuranes
M.D. Eggers, P.D. Livant and M.L. McKee (Auburn, AL, U.S.A.) 69
The role of hypervalent intermediates in alkyl transfer reactions at sulfonium centers
P.R. Young and B.P. Ruekberg (Chicago, IL, U.S.A.) 85
Some periodic trends in organic compounds containing O, S, Se, and Te: an ab initio study
V.K. Yadav, A. Yadav and R.A. Poirier (St. John's, Nfld., Canada) 101
Rotation-independent conjugation of sulfur–nitrogen bonds
P.G. Mezey and H. Flakus (Saskatoon, Sask., Canada) 117
Qualitative valence-bond descriptions of bonding for S–N, S–O, S–F and S–S compounds via increased-valence structures
R.D. Harcourt (Parkville, Vic., Australia) 131
Qualitative valence bond analysis of (10-S-4) sulfuranes and (9-S-3) sulfuranyl radicals
F. Volatron (Orsay, France) 167
The molecular structure of *p*-benzenedithiol as determined by electron diffraction
G. Portalone (Rome, Italy), A. Domenicano (L'Aquila, Italy), G. Schultz and I. Hargittai (Budapest, Hungary) 185
Sulfur-33 and oxygen-17 nuclear magnetic resonance spectroscopy of compounds containing –SO– and $-SO_2-$ moieties
G. Barbarella (Bologna, Italy) 197
Studies on conformation and configuration of *β*-hydroxysulphoxides
F. Alcudia, I. Fernández, J.M. Llera, M. Trujillo and F. Zorrilla (Seville, Spain) 211
Interactions between C=S groups in 1,2- and 1,3-*bis* (thiocarbonyl) compounds: a study by spectroscopy, X-ray crystallography, and CNDO/S calculations
L. Fälth, U. Håkansson and J. Sandström (Lund, Sweden) 239
Molecular structure of dithia dications and some aspects of their chemistry
H. Fujihara and N. Furukawa (Ibaraki, Japan) 261
Theoretical studies on transannular S–S interactions in geometrically constrained 1,5-dithiocane derivatives
R.S. Glass, L. Adamowicz and J.L. Broeker (Tucson, AZ, U.S.A.) 273
Reaction paths of circumambulatory rearrangements of sulfur-substituted cyclopentadienes
V.I. Minkin, R.M. Minyaev and J.A. Yudilevich (Rostov on Don, U.S.S.R.) 293

HO and HS substituent effect on alkyl radicals: an ab-initio molecular orbital study
J. Fossey and J. Sorba (Palaiseau, France) 305
Several unsolved problems of chemical behavior of the sulfur atom in organic sulfur chemistry
S. Oae (Okayama, Japan) 321
SINDO1 study of sulphur isomers and sulphur fluorine compounds
K. Jug and R. Iffert (Hannover, F.R.G.) 347

Author index 361

Subject index 362